ICTS
INTERNATIONAL CENTRE for THEORETICAL SCIENCES
TATA INSTITUTE OF FUNDAMENTAL RESEARCH

Computational Methods for Quantum Many-Body Physics

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Logistical details

- Class timings: Wednesdays 15:00-17:00
- Venue: Emmy Noether seminar room and online
- Zoom details:
  - Meeting ID: 876 3397 1378
  - Passcode: 171723
- Evaluation: Assignments (will be posted on the Moodle page)
- Contacts:
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    - All course material (slides, lecture notes, video recordings, and assignments) can be found at https://courses.icts.res.in/course/view.php?id=82

Purpose of this course

- obvious, introduce some the most commonly used numerical methods in many-body physics
- introduce how and why the methods work? understanding the algorithms behind methods
- how to extract useful and interesting physics from the numerical methods
- **understand the physics behind the algorithms**: If and how the algorithms work also encodes a lot of physics of the system under consideration
- At a practical level, lots of very well structured libraries available such as
  - ALPS [https://alpscore.org]
  - QuSpin [http://quspin.github.io/QuSpin/] [SciPost Phys. 2, 003 (2017), SciPost Phys. 7, 020 (2019)]
  - TenPY [https://tenpy.readthedocs.io/en/latest/][SciPost Phys. Lect. Notes 5 (2018)]
  - iTensor [https://itensor.org][SciPost Phys. Codebases 4 (2022)]
  - many many others $\cdots$

  Help understand how do the underlying algorithms in these packages so that they are no longer black boxes

Course Plan

- **Lectures 1-3: Exact diagonalisation**
  - representing Hamiltonians as sparse matrices
  - Lanczos algorithms for diagonalisation
  - Shift-invert and Polynomially filtered exact diagonalisation
  - time-evolution using ED
- **Lectures 4-7: Classical and Quantum Monte Carlo:**
  - Basic principles of Monte Carlo algorithms: importance sampling, detailed balance, autocorrelation timescales, error analysis
  - Illustrating classical Monte Carlo using the 2D Ising model: local, worm and cluster type algorithms
  - Some other useful tricks: parallel tempering, overrelaxation etc
  - Illustrating quantum Monte Carlo (QMC) using the 2D $S = 1/2$ Heisenberg antiferromagnet and the 2D J-Q model: Stochastic series expansion (SSE) QMC and its implementation
  - Introduction to sign problem (time permitting)
- **Lecture 8: Time-evolution of quantum systems**
  - (truncated) Krylov space methods
  - Kernel polynomial methods
- **Lectures 9-10: Tensor Network Methods**
  - matrix product states
  - matrix product operators
  - introduction to DMRG and tDMRG algorithms (time permitting)

Overview of the physics

Models: typically disordered, interacting quantum many-body Hamiltonians defined on regular, hierarchical or random lattices

- **Spin models**

$$H = \sum_{\langle i,j \rangle} \sum_{\mu,\nu=x,y,z} J_{ij}^{\mu\nu} \hat{S}_i^{\mu} \hat{S}_j^{\nu} + \sum_i \sum_{\mu=x,y,z} h_i^{\mu} \hat{S}_i^{\mu}$$

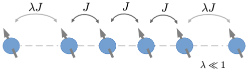
- **Fermi-Hubbard type models**

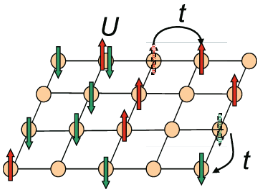
$$H = -t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} \epsilon_{i,\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- **Bose-Hubbard type models**

$$H = -t \sum_{\langle i,j \rangle} b_i^{\dagger} b_j + \sum_i \epsilon_{i,\sigma} b_i^{\dagger} b_i + \sum_{i,j} V_{ij} n_i n_j$$

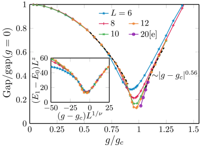
- many more: Bose-Fermi mixtures, $t-J$ models, electrons coupled to phonons, open quantum systems ...

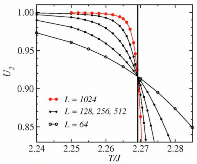


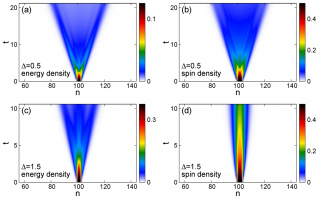


Overview of the Physics

- Eigenvalue spectrum
  - analysis of the gap across quantum phase transition
  - spectral correlations: ergodic, chaotic or integrable, localised
  - density of states, zero modes
- Correlation functions in ground states/eigenstates
  - correlation lengths: diverges across transition, long-range order
  - order parameters; scaling across QPTs
  - entanglement structure in the states
- Thermodynamic properties
  - partition functions and thermodynamic potentials
  - response functions, specific heat, susceptibilities
- Non-equilibrium dynamics
  - dynamical response, structure factors
  - non-equilibrium transport
  - quantum chaos or lack thereof







Schmitt et al., Sci. Adv. 2022; Sandvik's lecture note, Karrash et al. PRB 2014

Exact Diagonalisation

Basic structure of an ED code

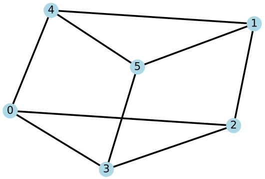
1. **Construct and enumerate the basis states**
   - label the sites of your lattice
   - enumerate the basis states ⇒ assign an unique integer label to each basis state
   - pick out the subset of basis states allowed by symmetries/conservation laws
2. **Construct the Hamiltonian as a matrix**
   - identify the diagonal elements of the Hamiltonian ⇒ these just associate numbers to each basis state
   - identify the off-diagonal terms in the Hamiltonian ⇒ for each term identify the set of basis states every basis state is connected to under the action of the term
3. **Diagonalise the Hamiltonian** ⇒ extract the required eigenvalues and eigenvectors
4. **Compute observabes**
   - express the operators of interest as matrices in the constructed basis
   - expectation values as matrix-vector multiplications

Simplest ED problem

Single particle hopping on some random lattice

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_i$$

- real-space basis a natural choice
- $|2\rangle = [0, 0, 1, 0, 0, 0]^\mathsf{T}$ is a basis state localised on site 2 of the lattice
- onsite potentials $\{\epsilon_i\}$ form the diagonal elements
- hopping between sites connected by lines constitute the off-diagonal elements



$$H = \begin{pmatrix} \epsilon_0 & 1 & 1 & 0 & 1 & 0 \\ 1 & \epsilon_1 & 1 & 0 & 0 & 1 \\ 1 & 1 & \epsilon_2 & 1 & 0 & 0 \\ 0 & 0 & 1 & \epsilon_3 & 1 & 1 \\ 1 & 0 & 0 & 1 & \epsilon_4 & 1 \\ 0 & 1 & 0 & 1 & 1 & \epsilon_5 . \end{pmatrix}$$

ED of an interacting spin-1/2 system: construction of basis

- **Interacting spin Hamiltonian on a 1D chain**

$$H = J\sum_{i=0}^{L-1}[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z] + \sum_i h_i\sigma_i^z$$

- **Computational basis**: classical configurations of σ^z-product states
- **Enumeration of the basis states**: spin-configurations → binary strings → integers

Configuration	String	Integer
$\uparrow\uparrow\uparrow\uparrow$	0000	0
$\uparrow\uparrow\uparrow\downarrow$	0001	1
$\uparrow\uparrow\downarrow\uparrow$	0010	2
$\uparrow\uparrow\downarrow\downarrow$	0011	3
$\uparrow\downarrow\uparrow\uparrow$	0100	4
$\vdots$	$\vdots$	$\vdots$
$\downarrow\downarrow\downarrow\downarrow$	1111	15

- Convert binary string $\{b_{L-1}, \cdots, b_1, b_0\}$ to an integer I:

$$I = \sum_{i=0}^{L-1} b_i 2^i$$

- Convert integer to I to binary string
  - at each step divide $I/2$: remainder forms the binary digit and update I to the quotient

Quotient	Binary
$7//2 = 3$	1
$3//2 = 1$	1
$1//2 = 0$	1
$0//2 = 0$	0

$$\begin{aligned} |7\rangle &= |0\cdots 0111\rangle \\ &= |\uparrow\cdots\uparrow\downarrow\downarrow\downarrow\rangle \end{aligned}$$

ED of an interacting spin-1/2 system: construction of Hamiltonian

- Identify the diagonal and off-diagonal components of the Hamiltonian in the computational basis

$$H_{\text{diag}} = J\sum_{i=0}^{L-1}[\sigma_i^z\sigma_{i+1}^z] + \sum_i h_i\sigma_i^z \qquad H_{\text{off-diag}} = J\sum_{i=0}^{L-1}[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y] = J\sum_{i=0}^{L-1}[\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+]$$

Diagonal part:

- Take state $|l\rangle = \{b_{L-1}^{(l)}, \cdots, b_1^{(l)}, b_0^{(l)}\}$
- Diagonal element $H_{ll} = \mathcal{E}_l$: the energy of the classical configuration

$$\mathcal{E}_l = J\sum_i (-1)^{b_i^{(l)}+b_i^{(l)}} + \sum_i h_i(-1)^{b_i^{(l)}}$$

Off-diagonal part:

- spin-flips, connect different spin configurations
- for each state $|l\rangle$, locate the states $|K\rangle$ for which $\langle K|H|l\rangle \neq 0$
- $H_{\text{off-diag}}$ flips nearest-neighbour anti-parallel spins
- for a given state $|l\rangle$, go to each site i

$$\text{XOR}(b_i^{(l)}, b_{i+1}^{(l)}) = \begin{cases} 1; & \text{if antiparallel} \\ 0; & \text{if parallel} \end{cases}$$

- if anti-parallel generate a new state

$$\{\cdots b_{i+1}^{(l)} b_i^{(l)} \cdots\} \Rightarrow \{\cdots b_i^{(l)} b_{i+1}^{(l)} \cdots\}$$

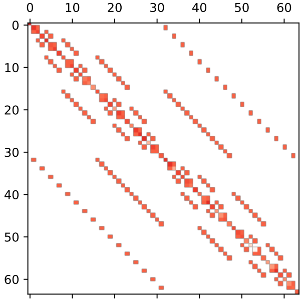
- generate the decimal representation of new binary string $\equiv K$ and set $H_{lK} = J$

ED of an interacting spin-1/2 system: What does the Hamiltonian look like?

Hamiltonian:

$$H = J\sum_{i=0}^{L-1}[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z] + \sum_i h_i\sigma_i^z$$

Plot of Hamiltonian matrix for $L = 6$



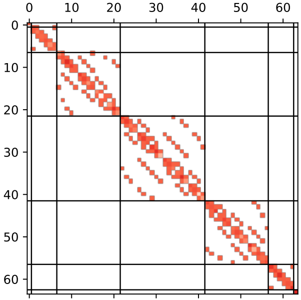
Conservation laws/Symmetries

- Total z-magnetisation $S^z = \sum_i \sigma_i^z$ is a conserved quantity:

$$[H, S^z] = 0$$

- Reorder the basis states to group them according to their S^z
- Hamiltonian becomes block diagonal
- Each block can be diagonalised separately

Hamiltonian in block diagonal form



ED of an interacting spin-1/2 system: Construct basis with symmetries

Why do we want to do this?

- Often, interested in problems with a fixed magnetisation, total particle number etc.
- If we do not treat each block separately, we can get spurious errors due to accidental near degenracies of eigenvalues, eigenstates mixed between different sectors
- Constructing the full matrix and slicing off the sector of interest is redundant
- Wastage of computational resources; can make the difference between being able and not being able to simulate beyond certain sizes

Comes at a cost

- We need to work a bit harder to efficiently enumerate the basis with symmetries

ED of an interacting spin-1/2 system: construction of basis with symmetries

Consider the sector with $S^z = 0$

Table of configurations and their decimal represetnations

Configuration	I	$J(I)$	Configuration	I	$J(I)$
000111	7	0	100011	35	10
001011	11	1	100101	37	11
001101	13	2	100110	38	12
001110	14	3	101001	41	13
010011	19	4	101010	42	14
010101	21	5	101100	44	15
010110	24	6	110001	49	16
011001	25	7	110010	50	17
011010	26	8	110100	52	18
011100	28	9	111000	56	19

Enumerating the basis

- brute force way is to assign indices in increasing order of the decimal representations of the binary strings
- makes it very inefficient:
  - for every decimal I, we have to search through the entire (sorted) list to find the appropriate $J(I)$
- two of the possible ways around
  - hashing functions
  - Lin tables Lin, PRB 1990

ED of an interacting spin-1/2 system: construction of basis with symmetries

Hashing functions

- associate the index of the basis state to the decimal representation of the binray string
- Example:

$$h(I) = [I(mod)\lambda] + 1$$

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001101	13	2	14	100110	38	12	16
001110	14	3	15	101001	41	13	19
010011	19	4	20	101010	42	14	20
010101	21	5	22	101100	44	15	22
010110	24	6	2	110001	49	16	4
011001	25	7	3	110010	50	17	5
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ED of an interacting spin-1/2 system: construction of basis with symmetries

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A general issue with hashing functions

- collisions: non-unique hashing values
- very difficult to avoid collisions

ED of an interacting spin-1/2 system: Lin Tables Lin PRB 1990

- basic idea is to not have a large 1D search
- split the lattice into two parts, A and B, and convert the search for the indices into a 2D search
- Define two integers, one for each part

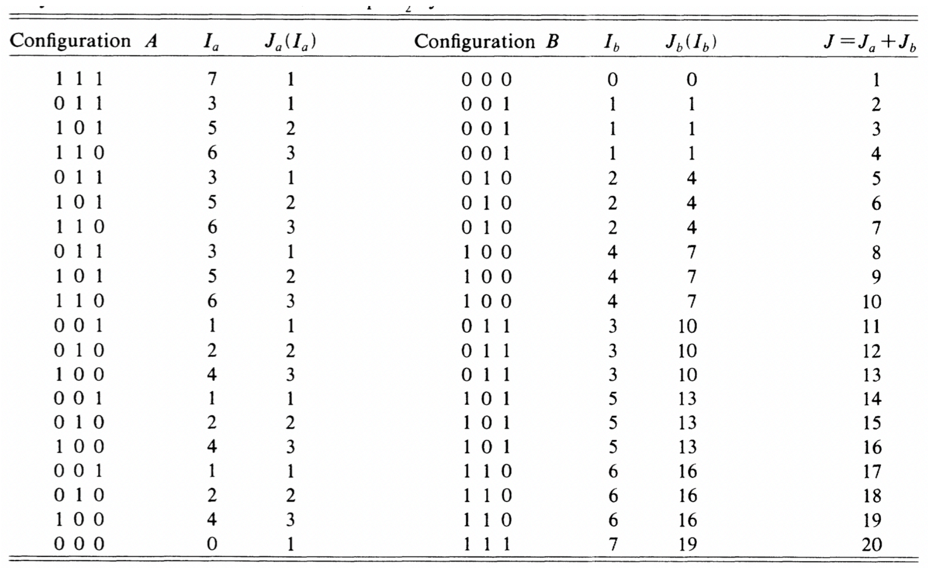
$$I_A = \sum_{i=0}^{L/2-1} b_i^{(I)} 2^i \qquad I_B = \sum_{i=0}^{L/2-1} b_{i+L/2}^{(I)} 2^i$$

- Define two vectors $J_A(I_A)$ and $J_B(I_B)$ so that the position of the configuration represented by integer I is given by

$$J = J_A(I_A) + J_B(I_B)$$

- maximum length of J_A and J_B is the square root of length of $J(I)$

ED of an interacting spin-1/2 system: Lin Tables Lin PRB 1990



Configuration A	I_a	$J_a(I_a)$	Configuration B	I_b	$J_b(I_b)$	$J=J_a+J_b$
1 1 1	7	1	0 0 0	0	0	1
0 1 1	3	1	0 0 1	1	1	2
1 0 1	5	2	0 0 1	1	1	3
1 1 0	6	3	0 0 1	1	1	4
0 1 1	3	1	0 1 0	2	4	5
1 0 1	5	2	0 1 0	2	4	6
1 1 0	6	3	0 1 0	2	4	7
0 1 1	3	1	1 0 0	4	7	8
1 0 1	5	2	1 0 0	4	7	9
1 1 0	6	3	1 0 0	4	7	10
0 0 1	1	1	0 1 1	3	10	11
0 1 0	2	2	0 1 1	3	10	12
1 0 0	4	3	0 1 1	3	10	13
0 0 1	1	1	1 0 1	5	13	14
0 1 0	2	2	1 0 1	5	13	15
1 0 0	4	3	1 0 1	5	13	16
0 0 1	1	1	1 1 0	6	16	17
0 1 0	2	2	1 1 0	6	16	18
1 0 0	4	3	1 1 0	6	16	19
0 0 0	0	1	1 1 1	7	19	20